STOCHASTIC PARAMETERIZATION FOR LARGE EDDY SIMULATION OF GEOPHYSICAL FLOWS

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ABSTRACT. Recently, stochastic, as opposed to deterministic, parameterizations are being investigated to model the effects of unresolved subgrid scales (SGS) in large eddy simulations (LES) of geophysical flows. We analyse such a stochastic approach in the barotropic vorticity equation to show that (i) if the stochastic parameterization approximates the actual SGS stresses, then the solution of the stochastic LES approximates the "true" solution at appropriate scale sizes; and that (ii) when the filter scale size approaches zero, the solution of the stochastic LES approaches the true solution.

1. MOTIVATION

The immense number of degrees of freedom in large scale turbulent flows as encountered in the world oceans and atmosphere makes it impossible to simulate these flows in all their detail in the foreseeable future. On the other hand, it is essential to represent these flows reasonably accurately in Ocean and Atmospheric General Circulation Models (OGCMs and AGCMs) so as to improve the confidence in these model components of the earth system in ongoing effort to study climate and its variability (e.g., see [1]). Furthermore, it is very often the case that in highly resolved computations, a rather disproportionately large fraction of the computational effort is expended on the small scales (e.g., see [5]) whereas a large fraction of the energy resides in the large scales (e.g., see [6]). It is for these reasons that the ideas of Large Eddy Simulation (LES)—wherein the large scale unsteady motions driven by specifics of the flow are explicitly computed, but the small (and presumably more universal [7]) scales are modelled—are natural in this context.

Given our interest in large scale geophysical flows with its small vertical to horizontal aspect ratio, we restrict ourselves to two-dimensional or quasi two-dimensional flows. Previous models of the small scales in how they affect the large scales in the momentum equations or equivalently the vorticity equation in incompressible settings have mostly been confined to an enhanced eddy viscosity or nonlinear eddy viscosity like that of Smagorinsky or biharmonic viscosity (e.g., see [8, 9, 10, 11, 12, 13]). Given the non-unique nature of the small scales with respect to the large scales [5], the aforementioned use of deterministic and dissipative

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closures seem rather highly restrictive. On the other hand, it would seem desirable to actually represent a population of eddies that satisfy overall constraints of the flow rather than make flow specific parametric assumptions. This has led to recent investigations of the possibility of using stochastic processes to model the effects of unresolved scales in geophysical flows (e.g., see [14, 15]). More recently, subgrid scale (SGS) stresses have been analysed in simple but resolved flows as a possible way to suggest stochastic parameterizations as e.g., in [3, 4, 30, 31]. These efforts have been preceded, of course, by various attempts to model anomalies in geophysical flow systems as linear Langevin equations (e.g., [28, 2, 16, 26]) and the analysis of stochastic models in isotropic and homogeneous three dimensional turbulence (e.g., [17, 18]).

In this paper, we analyze the stochastic approach to parameterization in the barotropic vorticity equation and show that (i) if the stochastic parameterization approximates the SGS stresses, then the stochastic large eddy solution approximates the "true" solution at appropriate scale sizes; and that (ii) when the filter scale size approaches zero, then the solution of the stochastic LES approaches the true solution. In the next section we present a set of computations that demonstrates the use of stochastic parameterizations and in §3, we prove the main results on approximation and convergence of LES solutions using stochastic parameterizations.

2. Stochastic parameterization

We consider the simple setting of the beta-plane barotropic vorticity equation (equivalently the two-dimensional (2D) quasi-geostrophic (QG) model) [27, 34]:

$$(2.1) q_t + J(\psi, q) + \beta \psi_x = f(x, y, t) + \nu \Delta q - rq,$$

on a bounded domain D with piecewise smooth boundary ∂D . Here the vorticity q(x,y,t) is given in terms of streamfunction $\psi(x,y,t)$ by $q=\Delta\psi$. β is the meridional gradient of the Coriolis parameter, $\nu > 0$ the viscous dissipation constant, r > 0 the Ekman dissipation constant and f(x, y, t) the wind forcing. The forcing f is always assumed to be mean-square integrable both in time and in space. In addition, $\Delta = \partial_{xx} + \partial_{yy}$ is the Laplacian operator in the plane and $J(h,g) = h_x g_y - h_y g_x$ is the Jacobian operator. The boundary condition (BC) is $q=0, \ \psi=0$ on ∂D and initial condition (IC) is $q(x, y, 0) = q_0(x, y)$.

Fine mesh simulations (q) are used to obtain the benchmark solution \bar{q} through convolution with a spatial filter $G_{\delta}(x,y)$, with spatial scale $\delta > 0$:

$$\bar{q}(x, y, t) := q * G_{\delta}$$

We use a Gaussian filter [19], $G_{\delta}(x,y) = \frac{1}{\pi\delta^2}e^{-\frac{(x^2+y^2)}{\delta^2}}$, where $\delta > 0$ is the filter size and the filter is such that (1) $q * G_{\delta}$ is infinitely differentiable in space and (2) $q * G_{\delta} \to q$ as $\delta \to 0$ in $L^2(D)$. Note that the Fourier transform of G_{δ} is $\widehat{G}_{\delta}(k_1, k_2) = e^{-\frac{\delta^2(k_1^2 + k_2^2)}{4}}, \text{ and that } \widehat{q*G}_{\delta}(k_1, k_2, t) = \widehat{G}_{\delta}(k_1, k_2)\widehat{q}(k_1, k_2, t).$ On convolving (2.1) with G_{δ} the large eddy solution \bar{q} is seen to satisfy

$$(2.3) \bar{q}_t + J(\bar{\psi}, \bar{q}) + \beta \bar{\psi}_x = \bar{f}(x, y, t) + \nu \Delta \bar{q} - r\bar{q} + R(q),$$

where the SGS stress term R(q) is defined as

(2.4)
$$R(q) := J(\bar{\psi}, \bar{q}) - \overline{J(\psi, q)}.$$

Note that since $\bar{q} \neq \bar{q}$, the SGS stress term R(q) above is more than the Reynolds stress and the SGS stress is usually further divided into three components, the explicit Leonard stress, and the cross stress and the SGS Reynolds stress that require further modeling. However, for our purposes, we will consider R(q) in its entirety. Since R(q) depends on q as well as \bar{q} , the equation (2.3) is not a closed system. We need to model or prescribe R(q) in terms of resolved quantity \bar{q} . On the other hand, R(q) may be explicitly diagnosed from a fully-resolved run, given the filter.

An analysis of R(q) reveals that its time-mean is much smaller than its standard deviation, and that its temporal behavior is highly irregular, leading to the possibility of approximating R(q) by a suitable stochastic process $\sigma(\bar{q},\omega)$ (defined on a probability space $(\Omega, \mathcal{F}, \mathbb{P})$, with $\omega \in \Omega$, the sample space, σ -field \mathcal{F} and probability measure \mathbb{P}). With such a putative stochastic closure, the LES model becomes a random partial differential equation (PDE) for $Q \sim \bar{q}$:

$$(2.5) Q_t + J(\Psi, Q) + \beta \Psi_x = \bar{f}(x, y, t) + \nu \Delta Q - rQ + \sigma(Q, \omega),$$

where $Q = \Delta \Psi$ and $\bar{f}(x,y,t) := f * G_{\delta}$, with BC: Q = 0, $\Psi = 0$ on ∂D and IC: $Q(x,y,0) = \bar{q}_0(x,y)$. Note that when the stochastic process $\sigma(Q,\omega)$ does not depend explicitly on Q—as is the case when for example, either R(q) or some of its statistical properties are used to construct $\sigma(\omega)$ —we end up with an additive stochastic closure. The more general case of the stochastic closure wherein there is an explicit dependence on the state of the system Q, corresponds to a multiplicative stochastic closure.

While one can get an idea of the stochastic forcing to be used to represent the effects of unresolved subgrid scales in the LES runs by analysing resolved runs at the scale of the LES computation, the selection of a specific functional form for the stochastic parameterization is beyond the scope of the present article. We aim at providing a quantitative guide to selecting the stochastic parameterization.

2.1. Numerical experiments. We now briefly present a set of computations using the beta-plane barotropic vorticity equation (2.1) in a rectangular midlatitude basin. Finite differencing in space is used along with Runge-Kutta time stepping, and other details of the setup may be found elsewhere [32]. The steady forcing is uniform in the zonal (x) directions and sinusoidal in the meridional (y) direction corresponding to a double-gyre wind forcing. At the parameter values that we are presently consider, the circulation is highly variable, but statistically stationary. We therefore consider long time averages over the attractor in place of ensemble averaging (over ω).

Fig. 1 shows the contour plots of the time average of streamfunction and potential vorticity as they emerge in the resolved computations. A discussion of the phenomenology of this circulation may be found in [32]. This simulation is then analysed using a Gaussian filter with a width that is four times the grid spacing of the resolved computations to obtain the SGS stress R(q).

Next we consider a pair of coarse-scale simulations in which the grid spacing is four times that of the resolved computation in both directions. Fig. 2 shows the time average of the streamfunction and potential vorticity as emerges from the coarse-scale computation when $\sigma(Q,\omega)$ in (2.5) is set to zero. The main differences, as compared to the resolved runs, clearly are the absence of the outer gyres in the

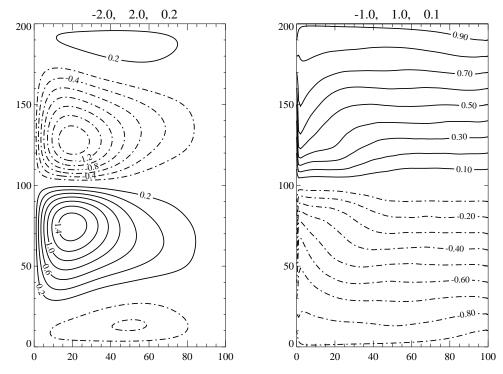


FIGURE 1. Resolved simulation. Contour plots of the average over the attractor (time-average) of streamfunction and potential-vorticity. Contour intervals are the same in all the figures and are indicated on top of the figures in the form (min, max, increment).

streamfunction field and the large amplitude grid scale oscillation in the potential vorticity field.

In the next case, we set the statistics of $\sigma(Q,\omega)$ (viz., its spatial and temporal correlation functions, amplitude and probability distribution function) identical to those of R(q) previously diagnosed from the resolved simulation. This we do by using the actual time history of the SGS stress R(q) in a coarse-resolution run in which the initial condition is slightly perturbed from the initial condition of the resolved run from which R(q) is diagnosed. Given the highly chaotic nature of the flow, the effect of the initial perturbation is to quickly lead to a complete decorrelation of the SGS stress forcing term R(q) from the state of the system Q. Thus, the actual time history of the diagnosed SGS stress R(q) supplied to the coarse-resolution run acts effectively as an additive stochastic closure $\sigma(\omega)$ of the SGS stresses in this LES. The time averages of the circulation for this case is shown in Fig. 3. Comparing Fig. 2 and Fig. 1 and Fig. 3 and Fig. 1, it is clear that the differences between the resolved case and the case with $\sigma(Q,\omega)$ similar to R(q) is much smaller than the differences between the resolved case and the case with $\sigma(Q,\omega)=0$.

These numerical experiments suggest that stochastic parameterizations can provide good representations of subgrid scales. So, the question then is as to how such an approach can be justified.

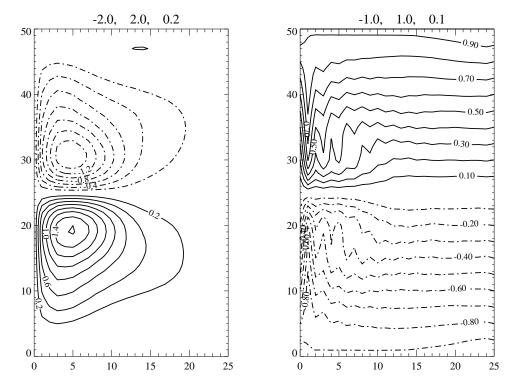


FIGURE 2. Coarse unresolved simulation. Contour plots of streamfunction and potential-vorticity, as in Fig. 1. The stochastic parameterization term $\sigma(Q,\omega)$ is set to 0.

In an attempt to answer this question, we will prove, following the approaches in [19, 29] in our stochastic context, that, under appropriate conditions on the stochastic parameterization (that appear easier to check in our case, c.f., Theorem 1 part (i) below and the Assumption A2 in [29]):

$$(2.6) \quad \mathbb{E}\|\bar{q} - Q\|^2 \quad \le \quad C(\nu, r, q_0, T) \cdot \quad \mathbb{E}\int_0^T \|R(q) - \sigma(Q, \omega)\|^2, \quad 0 \le t \le T,$$

(2.7)
$$\mathbb{E}||q - Q||^2 \to 0$$
, as $\delta \to 0$, $0 \le t \le T$.

where $C(\cdot) > 0$ is a constant, [0,T] is the computational time interval, $\mathbb{E}(Z(\omega)) := \int_{\Omega} Z(\omega) d\mathbb{P}(\omega)$, and $\|\cdot\|$ is the (spatial) norm in the space $L^2(D)$ of spatially mean-square integrable functions: $L^2(D) := \{f: \|f\| = \sqrt{\int_D f(x,y) dx dy} < \infty\}$.

3. Main results

Standard abbreviations $L^2=L^2(D),\, H_0^k=H_0^k(D),\, k=1,2,\ldots$, are used for the common Sobolev spaces in fluid mechanics [36, 22], with $<\cdot,\cdot>$ and $\|\cdot\|$ denoting the usual (spatial) scalar product and norm, respectively, in $L^2(D)$:

$$< f,g> := \int_D fg dx dy, \qquad \|f\| := \sqrt{< f,f>} = \sqrt{\int_D f(x,y) dx dy}.$$

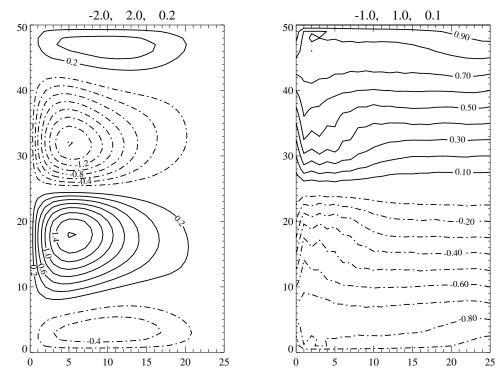


FIGURE 3. LES with stochastic parameterization. Contour plots of streamfunction and potential-vorticity, as in Fig. 1. The statistics of $\sigma(Q,\omega)$ are identical to those of R(q).

We need the following properties and estimates (see also [25, 20]) of the Jacobian operator $J: H_0^1 \times H_0^1 \to L^1$:

$$\begin{split} \int_D J(f,g)h\,dxdy &= -\int_D J(f,h)g\,dxdy, \int_D J(f,g)g\,dxdy = 0, \quad \text{and} \\ \left| \int_D J(f,g)\,dxdy \right| &\leq \|\nabla f\| \|\nabla g\| \quad \text{for all } f,\,g,\,h \in H^1_0, \\ \left| \int_D J(\Delta f,g)\Delta h\,dxdy \right| &\leq \sqrt{\frac{2|D|}{\pi}} \|\Delta f\| \; \|\Delta g\| \; \|\Delta h\| \quad \text{for all } f,\,g,\,h \in H^2_0. \end{split}$$

In addition, we recall the Poincaré, Young, and Gronwall inequalities below:

$$\begin{split} \|g\|^2 &= \int_D g^2(x,y) \, dx dy \leq \frac{|D|}{\pi} \int_D |\nabla g|^2 \, dx dy = \frac{|D|}{\pi} \|\nabla g\|^2 \quad \text{for } g \in H^1_0. \\ AB &\leq \frac{\epsilon}{2} A^2 + \frac{1}{2\epsilon} B^2 \quad \text{for } A, B \geq 0 \text{ and } \epsilon > 0. \end{split}$$

Assuming that $y(t) \geq 0$, g(t) and h(t) are integrable, if $\frac{dy}{dt} \leq gy + h$ for $t \geq t_0$, then

$$y(t) \le y(t_0)e^{\int_{t_0}^t g(\tau)d\tau} + \int_{t_0}^t h(s)e^{-\int_s^s g(\tau)d\tau}ds, \ t \ge t_0.$$

Lemma 3.1. ([20]) The quasi-geostrophic motion described by (2.1) satisfies the enstrophy estimate:

$$(3.1) ||q||^2 \leq ||q_0||^2 e^{-2\alpha t} + \frac{1}{r} \int_0^t ||f(s)||^2 e^{2\alpha(s-t)} ds, 0 \leq t < \infty$$

where $\alpha = \frac{r}{2} + \frac{\pi\nu}{|D|} - \frac{1}{2}|\beta| \left(\frac{|D|}{\pi} + 1\right)$ with |D| denoting the area of the domain D. Note that α is positive in the case of no rotation $(\beta = 0)$.

Theorem 3.2. (i) Stochastic Approximation:

If the stochastic paramerization $\sigma(Q,\omega)$ is such that

(3.3)
$$\int_0^T \|\sigma(Q,\omega)\|^2 dt \le M(T), \quad almost \ surely \ for \ \omega \in \Omega,$$

for some constant M > 0 depending on computational time interval, then

$$(3.4) \ \mathbb{E} \|\bar{q} - Q\|^2 \ \leq \ C(\nu, r, q_0, T) \cdot \ \mathbb{E} \int_0^T \|R(q) - \sigma(Q, \omega)\|^2 dt, \ 0 \leq t \leq T,$$

for any fixed time interval $0 \le t \le T$.

This implies that, if the stochastic paramerization $\sigma(Q, \omega)$ approximates the SGS stress R(q), then the LES solution Q approximates \bar{q} , in mean-square sense. (ii) **Scale convergence**: If the stochastic paramerization $\sigma(Q, \omega)$ satisfies

(3.5)
$$\mathbb{E} \int_0^T \|\sigma(Q,\omega)\|^2 dt \to 0, \quad as \ \delta \to 0,$$

for all LES solutions Q of 2.5), then

(3.6)
$$\mathbb{E}\|q - Q\|^2 \to 0$$
, as $\delta \to 0$, $0 < t < T$.

This implies that, if the stochastic paramerization $\sigma(Q,\omega)$ becomes smaller (collectively in computational time interval) as the cut-off scale size δ decreases, then the LES solution Q approximates the original solution q better, in mean-square sense.

Remark 3.3. Condition (3.3) means that the stochastic paramerization $\sigma(Q,\omega)$ is square-integrable in time and space, and its norm in the space $L^2((0,T);L^2(D))$ is almost surely bounded on the computational interval.

Remark 3.4. Condition (3.5) means that the variance of the stochastic paramerization $\sigma(q,\omega)$, collectively in the finite time interval of numerical simulation, becomes smaller and smaller as the cut-off scale size δ decreases.

To prove part (i), denote $U = \bar{q} - Q$, so that $U = \Delta(\bar{\psi} - \Psi)$. Note that U(0) = 0. Subtracting (2.3) from (2.5), we see that U satisfies

$$(3.7) \quad U_t = -J(\bar{\psi}, \bar{q}) + J(\Psi, Q) - \beta(\bar{\psi}_x - \Psi_x) + \nu \Delta U - rU + [R(q) - \sigma(Q, \omega)].$$

Multiplying this equation by U, integrating over D and noting that $\bar{q} = U + Q$, we obtain

(3.8)
$$\frac{1}{2}\frac{d}{dt}||U||^2 = -\int_D J(\bar{\psi} - \Psi, Q)U - \beta \int_D (\bar{\psi}_x - \Psi_x)U$$

(3.9)
$$-\nu \|\nabla U\|^2 - r\|U\|^2 + \int_D [R(q) - \sigma(Q, \omega)]U.$$

Note that, for $0 \le t \le T$,

$$\left| \int_{D} J(\bar{\psi} - \Psi, Q) U \, dx dy \right|$$

$$\leq \sqrt{\frac{2|D|}{\pi}} \|Q\| \|U\|^{2}$$

$$(3.10) \leq \sqrt{\frac{2|D|}{\pi}} \left\{ \|\bar{q}_{0}\|^{2} e^{2|\alpha|T} + \frac{1}{r} e^{2|\alpha|T} \int_{0}^{T} (\|\bar{f}(s)\|^{2} + \|\sigma(Q, \omega)\|^{2}) ds \right\} \|U\|^{2},$$

where we used the Lemma 3.1 on the LES model (2.5). Also, by the Young and Poincaré inequalities [36] we have

$$\left| \beta \int_{D} (\bar{\psi}_{x} - \Psi_{x}) U \, dx dy \right| \leq \frac{1}{2} |\beta| \left(\int_{D} (\bar{\psi}_{x} - \Psi_{x})^{2} \, dx dy + \int_{D} U^{2} \, dx dy \right)$$
$$\leq \frac{1}{2} |\beta| \left(\frac{|D|}{\pi} \int_{D} U^{2} \, dx dy + \int_{D} U^{2} \, dx dy \right),$$

that is

$$\left|\beta \int_{D} (\bar{\psi}_x - \Psi_x) U \, dx dy \right| \le \frac{1}{2} |\beta| \left(\frac{|D|}{\pi} + 1\right) ||U||^2.$$

Moreover,

$$(3.12) \qquad \left| \int_{D} [R(q) - \sigma(Q, \omega)] U \right| \le \frac{1}{2} \|R(q) - \sigma(Q, \omega)\|^2 + \frac{1}{2} \|U\|^2.$$

Putting all these estimates into (3.8), we obtain

$$\frac{d}{dt} \|U\|^{2} \leq 2 \left(-\alpha + \frac{1}{2} + \sqrt{\frac{2|D|}{\pi}}\right)
\left(\|\bar{q}_{0}\|^{2} e^{2|\alpha|T} + \frac{1}{r} e^{2|\alpha|T} \int_{0}^{T} \left[\|\bar{f}(s)\|^{2} + \|\sigma(Q, \omega)\|^{2}\right] ds\right) \|U\|^{2}
+ \|R(q) - \sigma(Q, \omega)\|^{2}.$$

Notice that α is defined in Lemma 3.1 in terms of physical parameters. By the Gronwall inequality [36] and noting U(0) = 0, we obtain

$$(3.14) \ \mathbb{E}\|\bar{q} - Q\|^2 = \mathbb{E}\|U\|^2 \le C(\nu, r, q_0, T) \cdot \mathbb{E}\int_0^t \|R(q) - \sigma(Q, \omega)\|^2 dt, \ 0 \le t \le T,$$

where C > 0 is a constant. This proves part (i) of Theorem 1.

To prove part (ii) of Theorem 1, denote V = q - Q, so that $V = \Delta(\psi - \Psi)$. Subtracting equation (2.1) from (2.5) leads to

(3.15)
$$V_t = -J(\psi, q) + J(\Psi, Q) - \beta(\psi_x - \Psi_x) + \nu \Delta V - rV + (f - \bar{f}) - \sigma(Q, \omega).$$

Similar to the approach in proving part (i) above, we estimate

$$\frac{d}{dt} \|V\|^{2} \leq 2 \left(-\alpha + 1 + \sqrt{\frac{2|D|}{\pi}} \right) \left(\|q_{0}\|^{2} e^{2|\alpha|T} + \frac{1}{r} e^{2|\alpha|T} \int_{0}^{T} \|f(s)\|^{2} ds \right) \|V\|^{2}
(3.16) + \|f - \bar{f}\|^{2} + \|\sigma(Q, \omega)\|^{2}.$$

By the Gronwall inequality again, we obtain

$$\mathbb{E}||V||^{2} \leq C_{1}(\nu, r, q_{0}, T) \mathbb{E}||q_{0} - \bar{q}_{0}||^{2}$$

$$+ C_{2}(\nu, r, q_{0}, T) \cdot \mathbb{E} \int_{0}^{T} \left[||f - \bar{f}||^{2} + ||\sigma(Q, \omega)||^{2} \right] dt, \quad 0 \leq t \leq T,$$

where C_1, C_2 are positive constants. Due to the property of G_{δ} , both $||q_0 - \bar{q}_0||$ and $||f - \bar{f}||$ go to zero as $\delta \to 0$. Together with the condition (3.5), we finally see that $\mathbb{E}||V||^2 = \mathbb{E}||q - Q||^2 \to 0$ as $\delta \to 0$, completing the proof of Theorem 1.

We view Theorem 1 as a starting point in our study of stochastic parameterization of SGS stress related terms in the LES of geophysical flows in the sense that it comments on the dependence of the LES solution only on the variance of the stochastic parameterization (its closeness to that of the actual SGS stress terms). Thus, it may be argued that the stochastic nature of the parameterization is not central to the results of this paper. However, to the extent that variance is one of the most fundamental characteristics of a stochastic process, understanding the dependence of the LES solution on it is important. What is now desirable is further characterization of the dependence of the LES solution on various other aspects of the stochastic parameterization such as its temporal and spatial correlation structure and its probability distribution function. These are subjects of ongoing research and we hope to report on them in the future.

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